

# ChemPhysChem

## Supporting Information

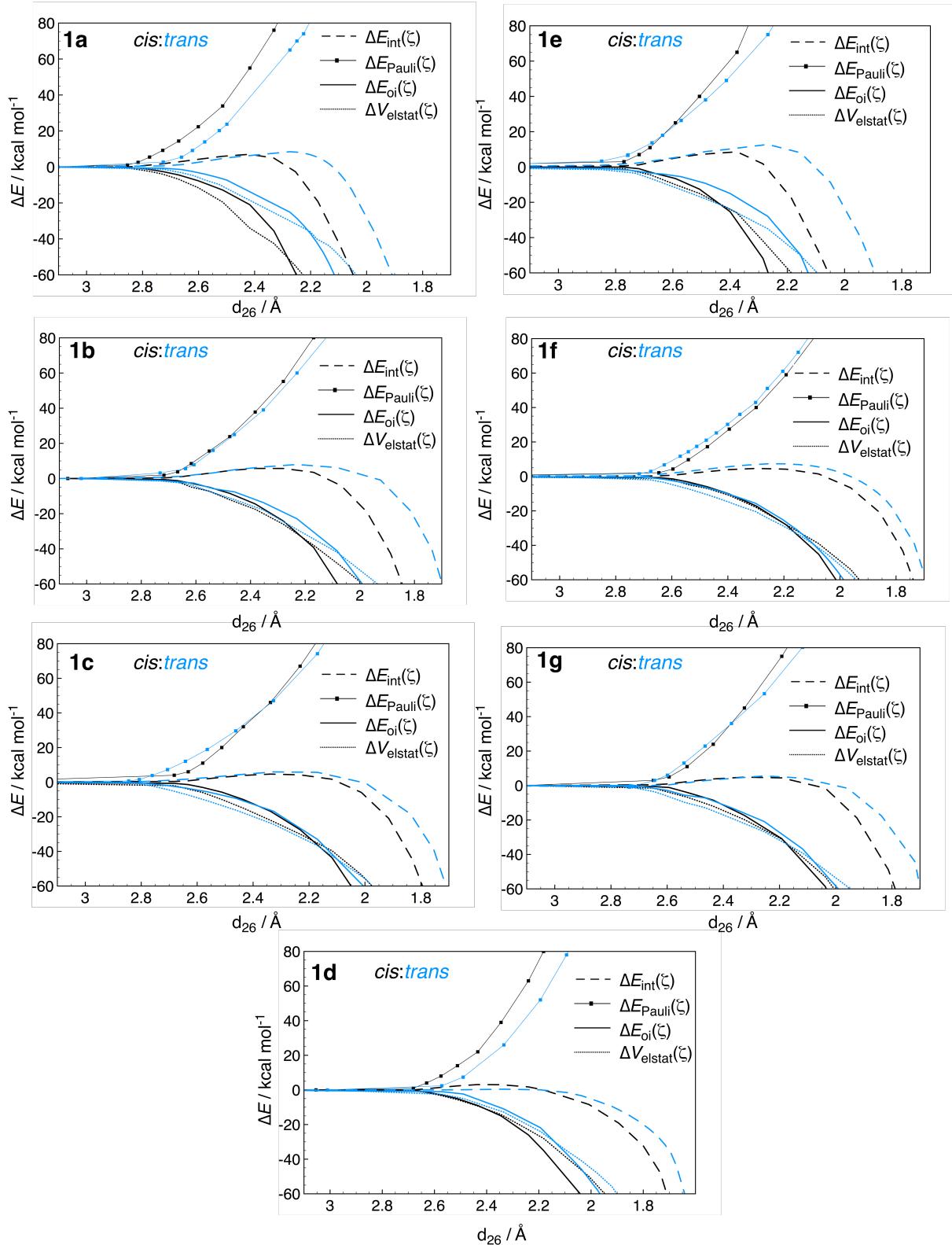
### Diastereoselectivity on Intramolecular Alder-ene Reaction of 1,6-Dienes

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<b>Table S1.</b> Activation strain analyses (in kcal mol <sup>-1</sup> ) and <HOMO <sub>ene</sub>   LUMO <sub>enophile</sub> > orbital overlap of transition structures associated with studied intramolecular ene–Alder reactions computed at M06-2X(PCM)/TZVP level for the C4–C5 fragmentation.....	S2
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**Table S1.** Activation strain analyses (in kcal mol<sup>-1</sup>) and  $\langle \text{HOMO}_{\text{ene}} | \text{LUMO}_{\text{enophile}} \rangle$  orbital overlap of transition structures associated with studied intramolecular ene–Alder reactions computed at M06-2X(PCM)/TZVP level for the C4–C5 fragmentation.

entry		<b>2</b>	$\Delta E_{\text{Pauli}}$	$\Delta V_{\text{elstat}}$	$\Delta E_{\text{oi}}$	$\Delta E_{\text{strain}}$			$\langle \text{HOMO}_{\text{ene}}   \text{LUMO}_{\text{enophile}} \rangle$
						[ene]	[enophile]	total	
1	<b>1a</b>	<i>cis</i>	138.5	-60.7	-95.2	33.8	16.7	50.5	0.212
2		<i>trans</i>	133.5	-58.0	-84.0	35.1	18.7	53.8	0.238
3	<b>1b</b>	<i>cis</i>	153.2	-72.1	-100.1	33.4	18.4	51.8	0.206
4		<i>trans</i>	182.8	-83.2	-116.2	33.0	24.5	57.5	0.291
5	<b>1c</b>	<i>cis</i>	159.9	-74.2	-103.7	32.0	22.3	54.3	0.207
6		<i>trans</i>	169.3	-76.6	-107.7	31.6	27.1	58.7	0.229
7	<b>1d</b>	<i>cis</i>	190.2	-90.5	-132.3	36.4	27.8	62.4	0.206
8		<i>trans</i>	238.4	-107.3	-171.1	35.2	35.6	70.8	0.225
9	<b>1e</b>	<i>cis</i>	159.5	-81.2	-90.8	39.3	17.5	56.8	0.143
10		<i>trans</i>	141.8	-62.3	-86.5	35.8	18.2	54.0	0.224
11	<b>1f</b>	<i>cis</i>	178.2	-84.8	-110.6	32.1	22.7	54.8	0.265
12		<i>trans</i>	183.5	-83.4	-114.1	32.2	22.3	53.5	0.273
13	<b>1g</b>	<i>cis</i>	158.0	-65.8	-177.6	30.4	17.1	47.5	0.209
14		<i>trans</i>	169.1	-79.5	-105.7	29.9	23.7	53.6	0.223



**Figure S1.** Energy decomposition analyses along the IRC projected the newly formed C–C bond ( $d_{26}$ ) of **1a–g** intramolecular ene–Alder reaction computed at ZORA-M062X/TZVP level of theory for the C4–C5 fragmentation

**Table S2.** Total electronic energies<sup>a</sup> (E, in a.u.), zero point correction of the energy<sup>b</sup> (ZPCE), thermal corrections to Gibbs free energies<sup>c</sup> (TCGFE, in a.u.), and number of imaginary frequencies<sup>d</sup> (NIMAG, in cm<sup>-1</sup>) of all stationary points discussed in the main text computed at M06-2X(PCM)/TZVP level.

Structure	E	ZPCE	TCGFE	NIMAG(v)
<b>1a</b>	-352.494851	0.228425 <sup>a</sup> (0.203951) <sup>b</sup>	0.191450 <sup>a</sup> (0.135617) <sup>b</sup>	0
<b>1a'</b>	-352.497544	0.228513 <sup>a</sup> (0.204030) <sup>b</sup>	0.191374 <sup>a</sup> (0.135425) <sup>b</sup>	0
<b>TSa-cis</b>	-352.436650	0.225366 <sup>a</sup> (0.201219) <sup>b</sup>	0.191974 <sup>a</sup> (0.139904) <sup>b</sup>	1 (-1214.1556)
<b>TSa-trans</b>	-352.431198	0.225244 <sup>a</sup> (0.201111) <sup>b</sup>	0.191281 <sup>a</sup> (0.138747) <sup>b</sup>	1 (-1291.5390)
<b>2a-cis</b>	-352.521702	0.231969 <sup>a</sup> (0.207115) <sup>b</sup>	0.197654 <sup>a</sup> (0.144019) <sup>b</sup>	0
<b>2a-trans</b>	-352.522840	0.231495 <sup>a</sup> (0.206692) <sup>b</sup>	0.196157 <sup>a</sup> (0.141846) <sup>b</sup>	0
<b>1b</b>	-580.377621	0.272986 <sup>a</sup> (0.243737) <sup>c</sup>	0.229879 <sup>a</sup> (0.142790) <sup>c</sup>	0
<b>1b'</b>	-580.378964	0.273051 <sup>a</sup> (0.243796) <sup>c</sup>	0.229576 <sup>a</sup> (0.142153) <sup>c</sup>	0
<b>TSb-cis</b>	-580.322232	0.269697 <sup>a</sup> (0.240801) <sup>c</sup>	0.229420 <sup>a</sup> (0.146677) <sup>c</sup>	1(-1142.0132)
<b>TSb-trans</b>	-580.322105	0.270118 <sup>a</sup> (0.241177) <sup>c</sup>	0.230077 <sup>a</sup> (0.147537) <sup>c</sup>	1 (-828.4293)
<b>2b-cis</b>	-580.397880	0.276217 <sup>a</sup> (0.246622) <sup>c</sup>	0.235489 <sup>a</sup> (0.151438) <sup>c</sup>	0
<b>2b-trans</b>	-580.400073	0.275992 <sup>a</sup> (0.246421) <sup>c</sup>	0.234876 <sup>a</sup> (0.150428) <sup>c</sup>	0
<b>1c</b>	-580.374159	0.273427 <sup>a</sup> (0.244131) <sup>c</sup>	0.229744 <sup>a</sup> (0.142191) <sup>c</sup>	0
<b>1c'</b>	-580.376277	0.273040 <sup>a</sup> (0.243786) <sup>c</sup>	0.230429 <sup>a</sup> (0.143755) <sup>c</sup>	0
<b>TSc-cis</b>	-580.318655	0.270103 <sup>a</sup> (0.241163) <sup>c</sup>	0.230110 <sup>a</sup> (0.147591) <sup>c</sup>	1 (-1106.4403)
<b>TSc-trans</b>	-580.319583	0.270240 <sup>a</sup> (0.241286) <sup>c</sup>	0.229183 <sup>a</sup> (0.145664) <sup>c</sup>	1 (-773.3642)
<b>2c-cis</b>	-580.395272	0.276499 <sup>a</sup> (0.246874) <sup>c</sup>	0.236376 <sup>a</sup> (0.152994) <sup>c</sup>	0
<b>2c-trans</b>	-580.397423	0.276160 <sup>a</sup> (0.246571) <sup>c</sup>	0.234826 <sup>a</sup> (0.150322) <sup>c</sup>	0
<b>1d</b>	-808.247532	0.316327 <sup>a</sup> (0.282435) <sup>c</sup>	0.266370 <sup>a</sup> (0.162657) <sup>c</sup>	0
<b>1d'</b>	-808.249166	0.316842 <sup>a</sup> (0.282895) <sup>c</sup>	0.267792 <sup>a</sup> (0.164886) <sup>c</sup>	0

<b>TSd</b> - <i>cis</i>	-808.192410	0.314475 <sup>a</sup> (0.280781) <sup>c</sup>	0.268138 <sup>a</sup> (0.169489) <sup>c</sup>	1 (-407.8655)
<b>TSd</b> - <i>trans</i>	-808.201994	0.314197 <sup>a</sup> (0.280533) <sup>c</sup>	0.267027 <sup>a</sup> (0.167691) <sup>c</sup>	1 (-614.7713)
<b>2d</b> - <i>cis</i>	-808.265573	0.319871 <sup>a</sup> (0.285599) <sup>c</sup>	0.271941 <sup>a</sup> (0.171048) <sup>c</sup>	0
<b>2d</b> - <i>trans</i>	-808.268427	0.319550 <sup>a</sup> (0.285313) <sup>c</sup>	0.271201 <sup>a</sup> (0.169701) <sup>c</sup>	0
<b>1e</b>	-431.114704	0.285060 <sup>a</sup>	0.244773 <sup>a</sup>	0
<b>1e'</b>	-431.118220	0.285237 <sup>a</sup>	0.245140 <sup>a</sup>	0
<b>TSe</b> - <i>cis</i>	-431.047852	0.281644 <sup>a</sup>	0.244014 <sup>a</sup>	1 (-1124.7357)
<b>TSe</b> - <i>trans</i>	-431.045862	0.281574 <sup>a</sup>	0.243945 <sup>a</sup>	1 (-1194.8127)
<b>2e</b> - <i>cis</i>	-431.129565	0.288715 <sup>a</sup>	0.250507 <sup>a</sup>	0
<b>2e</b> - <i>trans</i>	-431.135705	0.288708 <sup>a</sup>	0.250040 <sup>a</sup>	0
<b>1f</b>	-619.685900	0.301236 <sup>a</sup>	0.254956 <sup>a</sup>	0
<b>1f'</b>	-619.688446	0.301452 <sup>a</sup>	0.256737 <sup>a</sup>	0
<b>TSf</b> - <i>cis</i>	-619.627655	0.298451 <sup>a</sup>	0.257144 <sup>a</sup>	1 (-882.6807)
<b>TSf</b> - <i>trans</i>	-619.629814	0.298231 <sup>a</sup>	0.256286 <sup>a</sup>	1 (-777.8315)
<b>2f</b> - <i>cis</i>	-619.700894	0.304930 <sup>a</sup>	0.262788 <sup>a</sup>	0
<b>2f</b> - <i>trans</i>	-619.703644	0.304341 <sup>a</sup>	0.260150 <sup>a</sup>	0
<b>1g</b>	-619.684181	0.301110 <sup>a</sup>	0.256616 <sup>a</sup>	0
<b>1g'</b>	-619.680290	0.301441 <sup>a</sup>	0.257302 <sup>a</sup>	0
<b>TSg</b> - <i>cis</i>	-619.624420	0.298203 <sup>a</sup>	0.256577 <sup>a</sup>	1 (-1071.5289)
<b>TSg</b> - <i>trans</i>	-619.625362	0.298363 <sup>a</sup>	0.255982 <sup>a</sup>	1 (-732.2325)
<b>2g</b> - <i>cis</i>	-619.701278	0.305014 <sup>a</sup>	0.262791 <sup>a</sup>	0
<b>2a</b> - <i>trans</i>	-619.703830	0.304474 <sup>a</sup>	0.260476 <sup>a</sup>	0

<sup>a</sup>Computed at 298.15 K. <sup>b</sup>Computed at 453.15 K. <sup>c</sup>Computed at 528.15 K.

Cartesian coordinates (optimized at the M06-2X(PCM)/TZVP level) of all the stationary points collected in the main text

### 1a

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.492977	-1.699875	0.405863
2	6	0	-0.689098	-1.176100	-0.356214
3	6	0	-1.597096	-0.283169	0.034263
4	6	0	-1.598064	0.415769	1.362231
5	6	0	2.219337	0.187089	0.083759
6	6	0	1.350547	1.211740	-0.585915
7	6	0	0.891712	2.313392	-0.007659
8	6	0	-2.699679	0.156507	-0.889220
9	1	0	-0.789128	-1.581659	-1.362180
10	1	0	0.458795	-1.399665	1.454508
11	1	0	2.227838	0.366914	1.163255
12	1	0	3.246950	0.336221	-0.265844
13	1	0	-1.545324	1.497013	1.202036
14	1	0	1.091841	2.526431	1.037461
15	1	0	-2.598941	1.223294	-1.113106
16	1	0	-2.685613	-0.395989	-1.828311
17	1	0	-3.678656	0.022103	-0.421092
18	1	0	-2.527900	0.214258	1.901447
19	1	0	-0.760926	0.135202	1.997215
20	1	0	0.449207	-2.793258	0.396830
21	6	0	1.837447	-1.269636	-0.197089
22	1	0	1.819416	-1.437175	-1.279212
23	1	0	2.625515	-1.911789	0.203230
24	1	0	0.296640	3.035920	-0.552629
25	1	0	1.121789	1.027875	-1.633716

### 1a'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.350785	-1.252223	0.917450
2	6	0	-0.847221	-1.076372	0.031066
3	6	0	2.169760	0.977766	-0.074153
4	6	0	1.961487	-0.302647	-0.824837
5	6	0	-1.741042	-0.087319	0.029745
6	6	0	-1.732127	1.086021	0.970150
7	6	0	1.413500	2.059375	-0.202988
8	6	0	-2.887072	-0.080435	-0.946352
9	1	0	2.994015	0.987116	0.637070
10	1	0	-0.981728	-1.868305	-0.705592
11	1	0	0.482228	-0.391729	1.573670
12	1	0	1.150687	-0.169471	-1.545234
13	1	0	2.866182	-0.544117	-1.390598
14	1	0	-2.849917	0.813017	-1.576274
15	1	0	-2.612917	1.053731	1.618200
16	1	0	-1.791165	2.020170	0.404650
17	1	0	-0.844362	1.128590	1.596113
18	1	0	-3.844021	-0.053665	-0.417522
19	1	0	-2.873782	-0.958496	-1.591440
20	1	0	0.194705	-2.121910	1.563953
21	6	0	1.634068	-1.474829	0.108017
22	1	0	2.469036	-1.638633	0.795111
23	1	0	1.533526	-2.385477	-0.489286
24	1	0	1.598357	2.958349	0.372259
25	1	0	0.576325	2.074813	-0.893662

### TSa-cis

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	0.989679	-1.402098	0.498427
2	6	0	-0.174133	-0.930012	-0.331833
3	6	0	-1.442001	-0.595038	0.116655
4	6	0	-1.609491	0.075952	1.335385
5	6	0	2.042293	0.699588	-0.138320
6	6	0	0.647412	1.064695	-0.603097
7	6	0	-0.091934	2.002980	0.137142
8	6	0	-2.520311	-0.396152	-0.916925
9	1	0	-0.122597	-1.289605	-1.358311
10	1	0	0.896309	-1.071183	1.535412
11	1	0	2.178587	1.087717	0.875388
12	1	0	2.784389	1.193904	-0.771322
13	1	0	-0.984094	1.224815	0.880052
14	1	0	0.408670	2.499027	0.963469
15	1	0	-2.477068	0.635576	-1.291646
16	1	0	-2.394829	-1.065936	-1.767612
17	1	0	-3.514725	-0.548651	-0.495540
18	1	0	-2.611743	0.363661	1.636362
19	1	0	-0.941685	-0.138465	2.163182
20	1	0	1.026095	-2.494760	0.504495
21	6	0	2.254412	-0.812096	-0.116916
22	1	0	2.367749	-1.190736	-1.137374
23	1	0	3.154936	-1.085406	0.435790
24	1	0	-0.810715	2.626907	-0.384831
25	1	0	0.465162	1.006224	-1.670617

### TSa-trans

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.943188	-1.528758	-0.184095
2	6	0	-0.089408	-0.538980	-0.641259
3	6	0	0.607698	0.958316	0.577422
4	6	0	1.999701	0.741237	0.027178
5	6	0	-1.435608	-0.497294	-0.324195
6	6	0	-1.965517	-1.246459	0.866881
7	6	0	-0.148636	2.118679	0.382146
8	6	0	-2.132771	0.631095	-0.816632
9	1	0	0.440311	0.441167	1.521804
10	1	0	0.177304	-0.026854	-1.564412
11	1	0	0.664819	-1.928484	0.793259
12	1	0	2.076051	1.233485	-0.945425
13	1	0	2.734365	1.221307	0.678232
14	1	0	-1.384280	1.555534	-0.224512
15	1	0	-3.045711	-1.136481	0.952539
16	1	0	-1.515815	-0.868514	1.793678
17	1	0	-1.734529	-2.310917	0.807653
18	1	0	-3.168238	0.769273	-0.519898
19	1	0	-1.933919	0.931718	-1.841958
20	1	0	1.018029	-2.377240	-0.867750
21	6	0	2.289743	-0.771027	-0.093915
22	1	0	2.860792	-1.123011	0.765849
23	1	0	2.901340	-0.966085	-0.975638
24	1	0	-0.690785	2.542064	1.219846
25	1	0	0.189915	2.842192	-0.354463

### 2a-cis

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.733108	-1.416986	0.044222
2	6	0	-0.140107	-0.293699	-0.530204
3	6	0	-1.592845	-0.271457	-0.132928
4	6	0	-2.165894	-1.202083	0.624838
5	6	0	2.083408	0.570448	-0.525417
6	6	0	0.649528	0.989384	-0.178169

7	6	0	0.513042	1.369154	1.293912
8	6	0	-2.381785	0.886395	-0.683406
9	1	0	-0.115324	-0.372128	-1.625964
10	1	0	0.485796	-1.578041	1.094643
11	1	0	2.829094	1.206411	-0.045805
12	1	0	2.231467	0.648713	-1.604696
13	1	0	0.878590	0.568940	1.941887
14	1	0	1.096173	2.265571	1.511794
15	1	0	-2.019832	1.833668	-0.275031
16	1	0	-2.267897	0.945762	-1.769211
17	1	0	-3.441584	0.794463	-0.448894
18	1	0	-3.220627	-1.148477	0.868843
19	1	0	-1.615217	-2.046589	1.018188
20	1	0	0.568614	-2.363089	-0.471775
21	6	0	2.189004	-0.907887	-0.083987
22	1	0	2.759500	-1.491806	-0.805949
23	1	0	2.708506	-0.993840	0.870797
24	1	0	-0.526359	1.562665	1.565952
25	1	0	0.324353	1.828158	-0.797937

## 2a-trans

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.590956	-1.571666	-0.083591
2	6	0	-0.114811	-0.247309	-0.438006
3	6	0	0.745991	0.806747	0.274756
4	6	0	2.162724	0.325740	-0.044878
5	6	0	-1.584631	-0.211582	-0.109006
6	6	0	-1.964211	-0.131984	1.345165
7	6	0	0.444425	2.234015	-0.147369
8	6	0	-2.507166	-0.237772	-1.067162
9	1	0	0.586837	0.702862	1.355116
10	1	0	-0.003766	-0.077212	-1.515486
11	1	0	0.196101	-1.962535	0.856188
12	1	0	2.406764	0.617907	-1.070953
13	1	0	2.916349	0.767844	0.608175
14	1	0	-0.591161	2.501672	0.075127
15	1	0	-3.035637	-0.275732	1.478538
16	1	0	-1.697630	0.845031	1.757258
17	1	0	-1.437616	-0.881643	1.939855
18	1	0	-3.566085	-0.229922	-0.835943
19	1	0	-2.228952	-0.270270	-2.114368
20	1	0	0.413365	-2.331091	-0.844727
21	6	0	2.090704	-1.210317	0.072434
22	1	0	2.461590	-1.538739	1.043930
23	1	0	2.706227	-1.697567	-0.683415
24	1	0	1.096536	2.946448	0.361260
25	1	0	0.593180	2.347718	-1.224613

## 1b

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.304206	1.585696	1.425872
2	6	0	-0.965661	1.749486	0.088067
3	6	0	-0.248555	2.693107	-0.839037
4	6	0	-2.071598	1.113914	-0.298767
5	6	0	-2.909159	0.126578	0.463148
6	6	0	-2.973763	-1.247470	-0.220044
7	6	0	-1.736856	-2.119709	0.028672
8	6	0	-0.463691	-1.496065	-0.439085
9	6	0	0.639629	-1.382424	0.294414
10	6	0	1.828878	-0.700924	-0.248851
11	8	0	2.817422	-0.645290	0.659976
12	6	0	4.000126	0.037854	0.243086
13	8	0	1.931213	-0.221029	-1.352400
14	1	0	-0.442905	-1.104399	-1.453441
15	1	0	-2.434331	1.318144	-1.305330

16	1	0	-2.556172	0.004510	1.488812
17	1	0	-1.658641	-2.359475	1.092324
18	1	0	-1.871091	-3.066799	-0.504983
19	1	0	0.744289	1.300371	1.290750
20	1	0	0.696512	-1.731869	1.318162
21	1	0	0.750996	2.310229	-1.064145
22	1	0	-0.785660	2.820929	-1.778357
23	1	0	-0.124048	3.674432	-0.372765
24	1	0	-0.303939	2.536231	1.966884
25	1	0	-0.775841	0.832539	2.052649
26	1	0	4.686041	-0.016702	1.082608
27	1	0	4.428767	-0.444241	-0.634384
28	1	0	3.771765	1.075977	0.002712
29	1	0	-3.926998	0.522451	0.531541
30	1	0	-3.110001	-1.108494	-1.297022
31	1	0	-3.848683	-1.793532	0.138533

### 1b'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.522184	0.484740	-0.186074
2	6	0	-0.108729	-1.752665	0.394267
3	6	0	1.261383	-2.001194	0.931902
4	6	0	2.309096	-0.737842	-1.029842
5	6	0	-0.850915	-0.691549	0.693008
6	6	0	-2.172420	-0.488063	0.064969
7	8	0	-2.698227	-1.221140	-0.736505
8	6	0	1.773044	1.585783	-0.120537
9	6	0	2.134248	2.713002	0.809457
10	6	0	0.532825	1.840109	-0.932286
11	8	0	-2.740141	0.651860	0.490385
12	6	0	-4.017721	0.953404	-0.073220
13	1	0	-0.507163	-2.471996	-0.318985
14	1	0	3.400271	0.441155	0.457956
15	1	0	1.373247	-0.670635	-1.585419
16	1	0	1.512991	-1.226935	1.659337
17	1	0	1.277973	-2.964022	1.450449
18	1	0	1.326509	2.891563	1.525329
19	1	0	-0.507448	0.073544	1.379279
20	1	0	0.682254	2.710025	-1.578293
21	1	0	-0.307501	2.076313	-0.272707
22	1	0	0.243357	0.997571	-1.556087
23	1	0	2.273233	3.643928	0.252833
24	1	0	3.047909	2.502488	1.364572
25	1	0	-4.325195	1.892850	0.375211
26	1	0	-3.940184	1.052486	-1.155199
27	1	0	-4.731269	0.164906	0.162139
28	1	0	3.109597	-0.812115	-1.772556
29	6	0	2.309529	-2.022280	-0.190463
30	1	0	2.127913	-2.878941	-0.844582
31	1	0	3.295296	-2.168619	0.258604

### TSb-cis

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.302887	1.455638	1.482158
2	6	0	-0.885893	1.659115	0.216485
3	6	0	-0.259315	2.623762	-0.751301
4	6	0	-1.781241	0.704645	-0.280567
5	6	0	-2.878460	0.023645	0.507375
6	6	0	-3.109896	-1.309475	-0.193189
7	6	0	-1.725136	-1.952138	-0.256940
8	6	0	-0.651196	-0.896730	-0.512454
9	6	0	0.483194	-0.934424	0.339553
10	6	0	1.760990	-0.468024	-0.179525
11	8	0	2.810448	-0.902193	0.552114
12	6	0	4.087401	-0.419688	0.140954

13	8	0	1.901503	0.274378	-1.130061
14	1	0	-0.422081	-0.688463	-1.553006
15	1	0	-2.087363	0.882286	-1.311080
16	1	0	-2.572634	-0.149542	1.541839
17	1	0	-1.516422	-2.428554	0.703769
18	1	0	-1.668898	-2.729595	-1.020991
19	1	0	0.298021	0.366250	1.158839
20	1	0	0.526350	-1.656645	1.144879
21	1	0	0.704796	2.982675	-0.394083
22	1	0	-0.109747	2.153162	-1.724240
23	1	0	-0.916982	3.486549	-0.891283
24	1	0	0.433521	2.176358	1.822782
25	1	0	-0.920016	1.052440	2.279889
26	1	0	4.806468	-0.863741	0.823054
27	1	0	4.300262	-0.720980	-0.884115
28	1	0	4.124993	0.667564	0.204563
29	1	0	-3.776909	0.644348	0.522512
30	1	0	-3.494892	-1.125557	-1.200030
31	1	0	-3.829440	-1.943999	0.324987

### TSb-trans

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.773393	0.415015	0.525691
2	6	0	0.603243	-0.832016	-0.079704
3	6	0	1.564383	-2.002065	0.092862
4	6	0	2.948061	0.015404	-0.335634
5	6	0	-0.660277	-0.833769	0.579049
6	6	0	-1.818145	-0.382074	-0.159078
7	8	0	-1.793261	0.309023	-1.163107
8	6	0	1.030381	1.604138	0.396136
9	6	0	0.026559	1.781724	1.381863
10	6	0	0.988765	2.335073	-0.906928
11	8	0	-2.987172	-0.761254	0.412592
12	6	0	-4.166245	-0.284268	-0.228380
13	1	0	0.520618	-0.525041	-1.123025
14	1	0	1.877827	0.080744	1.558358
15	1	0	2.796009	0.376959	-1.354491
16	1	0	1.541699	-2.328844	1.134674
17	1	0	1.230450	-2.843611	-0.515058
18	1	0	-0.575616	0.710716	1.189766
19	1	0	-0.834826	-1.481787	1.428969
20	1	0	0.266428	3.148309	-0.882676
21	1	0	0.703523	1.653263	-1.715577
22	1	0	1.972327	2.742080	-1.153037
23	1	0	-0.654742	2.618236	1.262109
24	1	0	0.325804	1.610538	2.413735
25	1	0	-4.998024	-0.672675	0.352517
26	1	0	-4.186832	0.805445	-0.237308
27	1	0	-4.220910	-0.645722	-1.254875
28	1	0	3.879174	0.450668	0.029386
29	6	0	2.979236	-1.528966	-0.308496
30	1	0	3.266455	-1.923864	-1.282486
31	1	0	3.717981	-1.886747	0.408857

### 2b-cis

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.470318	1.770855	1.270432
2	6	0	-0.153688	1.663897	0.100254
3	6	0	0.330751	2.400839	-1.118208
4	6	0	-1.362369	0.791991	-0.136025
5	6	0	-2.214931	0.395802	1.080259
6	6	0	-2.979466	-0.881111	0.651637
7	6	0	-2.429139	-1.250203	-0.742891
8	6	0	-1.059094	-0.567063	-0.819861

9	6	0	0.001156	-1.369472	-0.065996
10	6	0	1.403912	-0.876656	-0.313008
11	8	0	2.195567	-1.056219	0.752070
12	6	0	3.538908	-0.593600	0.603557
13	8	0	1.802720	-0.418179	-1.353597
14	1	0	-0.725911	-0.432568	-1.849873
15	1	0	-2.013246	1.330887	-0.834891
16	1	0	-1.584690	0.178912	1.942268
17	1	0	-2.373071	-2.327607	-0.904150
18	1	0	-3.073211	-0.835877	-1.521057
19	1	0	-0.182587	-1.381388	1.009275
20	1	0	-0.019148	-2.409914	-0.405673
21	1	0	1.249468	2.950106	-0.914780
22	1	0	0.523182	1.700703	-1.933782
23	1	0	-0.431029	3.107549	-1.458549
24	1	0	1.354809	2.389924	1.368843
25	1	0	0.137355	1.256713	2.162382
26	1	0	4.032213	-0.804852	1.547158
27	1	0	4.034835	-1.114725	-0.214084
28	1	0	3.541826	0.477183	0.400267
29	1	0	-2.878794	1.208680	1.373446
30	1	0	-4.056801	-0.721669	0.621975
31	1	0	-2.799635	-1.688555	1.362536

## 2b-trans

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.233815	0.456148	0.500099
2	6	0	0.945000	-0.858534	-0.250465
3	6	0	2.218375	-1.674727	0.007591
4	6	0	2.678117	0.744868	0.073821
5	6	0	-0.330827	-1.557789	0.195854
6	6	0	-1.570163	-0.859403	-0.305394
7	8	0	-1.698454	-0.400408	-1.412301
8	6	0	0.229499	1.553961	0.262228
9	6	0	-0.629601	1.906365	1.215976
10	6	0	0.214565	2.204194	-1.093272
11	8	0	-2.545571	-0.833555	0.610605
12	6	0	-3.738105	-0.151523	0.217597
13	1	0	0.865518	-0.639361	-1.319555
14	1	0	1.230089	0.216586	1.570835
15	1	0	2.679810	1.143627	-0.943096
16	1	0	2.115300	-2.207012	0.957098
17	1	0	2.384000	-2.424919	-0.766118
18	1	0	-0.372753	-1.635820	1.283637
19	1	0	-0.361606	-2.573909	-0.209969
20	1	0	-0.651394	2.856363	-1.199769
21	1	0	0.172848	1.453466	-1.884945
22	1	0	1.115988	2.802169	-1.246818
23	1	0	-1.377831	2.672651	1.047796
24	1	0	-0.611835	1.437604	2.193516
25	1	0	-4.413003	-0.220296	1.065002
26	1	0	-3.510471	0.889993	-0.008654
27	1	0	-4.175646	-0.622379	-0.661526
28	1	0	3.166686	1.477268	0.716855
29	6	0	3.365223	-0.637145	0.096949
30	1	0	4.071267	-0.741230	-0.726380
31	1	0	3.929831	-0.771586	1.019748

## 1c

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.560213	1.078170	-1.104404
2	6	0	-2.787842	0.810162	-0.284925

3	6	0	-3.422277	-0.346898	-0.093205
4	6	0	-4.643441	-0.425783	0.783307
5	6	0	-3.028218	-1.662019	-0.708621
6	6	0	-0.051185	0.922178	0.965970
7	6	0	0.279253	-0.496698	0.616033
8	6	0	1.458058	-0.995517	0.240284
9	1	0	-0.552514	-1.196029	0.655161
10	1	0	-3.188876	1.686113	0.224223
11	1	0	-1.181046	0.162384	-1.559531
12	1	0	0.798229	1.406341	1.444130
13	1	0	-0.890070	0.912315	1.664945
14	1	0	-2.873325	-2.412083	0.072575
15	6	0	2.694062	-0.196403	0.115761
16	1	0	-5.501423	-0.796726	0.215648
17	1	0	-4.482260	-1.127637	1.606395
18	1	0	-4.901749	0.545740	1.203346
19	1	0	-3.836758	-2.035684	-1.342988
20	1	0	-2.125316	-1.605563	-1.312481
21	8	0	3.754622	-0.992993	-0.099111
22	8	0	2.788767	1.005654	0.183282
23	6	0	5.009238	-0.326186	-0.242954
24	1	0	5.742276	-1.108289	-0.413667
25	1	0	4.978862	0.361188	-1.087443
26	1	0	5.248519	0.231431	0.661589
27	1	0	-1.817066	1.749979	-1.929270
28	6	0	-0.446775	1.734999	-0.277709
29	1	0	0.439017	1.872013	-0.900545
30	1	0	-0.770535	2.726634	0.049606
31	1	0	1.562966	-2.049440	0.017716

### 1c'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.598574	0.157201	0.588636
2	6	0	-1.884520	1.247024	-0.154700
3	6	0	-0.611677	-2.115740	0.337841
4	6	0	-1.466026	-1.659131	-0.800370
5	6	0	-0.741655	1.855009	0.159845
6	6	0	0.061667	1.599294	1.404607
7	6	0	0.651079	-1.799364	0.626024
8	6	0	-0.137717	2.888343	-0.750951
9	1	0	-1.108173	-2.787579	1.036917
10	1	0	-2.360781	1.538282	-1.090302
11	1	0	-2.057468	-0.121335	1.494425
12	1	0	-0.939533	-0.926208	-1.406559
13	1	0	-1.676445	-2.528753	-1.431912
14	1	0	0.823959	2.529710	-1.130405
15	6	0	1.511633	-0.896725	-0.168305
16	1	0	0.045095	2.482592	2.049847
17	1	0	1.109803	1.424177	1.145139
18	1	0	-0.289421	0.747137	1.981965
19	1	0	0.052684	3.820865	-0.212308
20	1	0	-0.782408	3.103372	-1.602535
21	8	0	2.663658	-0.661792	0.489029
22	8	0	1.277956	-0.414579	-1.249084
23	6	0	3.580738	0.210345	-0.170447
24	1	0	4.442820	0.285843	0.484759
25	1	0	3.867935	-0.200094	-1.137575
26	1	0	3.129197	1.191311	-0.321983
27	1	0	-3.582434	0.514454	0.908236
28	6	0	-2.794238	-1.084373	-0.292044
29	1	0	-3.338352	-1.847980	0.271403
30	1	0	-3.413681	-0.823757	-1.154026
31	1	0	1.120036	-2.202379	1.514546

### TSc-cis

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z

1	6	0	1.303142	1.259635	1.173439
2	6	0	1.958953	0.309705	0.197768
3	6	0	2.082222	-1.069528	0.407753
4	6	0	2.942241	-1.864961	-0.528315
5	6	0	1.042234	-1.740150	1.085897
6	6	0	0.376596	1.919478	-1.018128
7	6	0	0.581458	0.400414	-1.129302
8	6	0	-0.487711	-0.510695	-0.878329
9	1	0	1.160466	0.111295	-2.001822
10	1	0	2.780106	0.767537	-0.353263
11	1	0	0.436032	0.790340	1.636420
12	1	0	-0.671208	2.157175	-1.188830
13	1	0	0.952267	2.386902	-1.817758
14	1	0	0.140652	-1.416783	0.245970
15	6	0	-1.699327	-0.111033	-0.181019
16	1	0	3.375400	-2.734955	-0.034495
17	1	0	2.322896	-2.237325	-1.355584
18	1	0	3.743251	-1.262398	-0.954561
19	1	0	1.096204	-2.823545	1.136692
20	1	0	0.625220	-1.286077	1.979048
21	8	0	-2.714907	-0.979144	-0.402454
22	8	0	-1.834684	0.849960	0.550339
23	6	0	-3.926483	-0.696971	0.292165
24	1	0	-4.620912	-1.482801	0.009454
25	1	0	-3.763067	-0.704609	1.369590
26	1	0	-4.318246	0.277349	0.002020
27	1	0	1.998756	1.548335	1.964300
28	6	0	0.836621	2.461196	0.353050
29	1	0	0.029095	2.987455	0.859120
30	1	0	1.661728	3.164141	0.220672
31	1	0	-0.611585	-1.351092	-1.549930

### TSc-trans

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.620557	-0.871789	-0.593004
2	6	0	-1.454380	0.093869	-0.610922
3	6	0	-0.496487	-0.544772	0.820829
4	6	0	-0.636807	-1.999178	0.373349
5	6	0	-1.562860	1.467292	-0.337400
6	6	0	-2.705296	2.015494	0.460837
7	6	0	0.765080	0.096989	0.991761
8	6	0	-0.358449	2.206027	-0.487216
9	1	0	-1.164498	-0.344777	1.661243
10	1	0	-0.710830	-0.140991	-1.372281
11	1	0	-3.431234	-0.478793	0.021981
12	1	0	0.030691	-2.179411	-0.467404
13	1	0	-0.336910	-2.659332	1.189075
14	1	0	0.330301	1.569277	0.308252
15	6	0	1.870094	-0.167940	0.101507
16	1	0	-2.512511	3.039412	0.776020
17	1	0	-2.894615	1.406757	1.350500
18	1	0	-3.625950	2.006874	-0.128115
19	1	0	-0.373562	3.255862	-0.211006
20	1	0	0.217754	2.004346	-1.389356
21	8	0	3.052673	0.278109	0.593226
22	8	0	1.793973	-0.666676	-1.008703
23	6	0	4.172822	0.129921	-0.273466
24	1	0	5.022805	0.536419	0.267194
25	1	0	4.341846	-0.920421	-0.509147
26	1	0	4.017974	0.678159	-1.202566
27	1	0	-3.017188	-0.992381	-1.601852
28	6	0	-2.103083	-2.214332	-0.017507
29	1	0	-2.687122	-2.489585	0.861965
30	1	0	-2.204908	-3.028519	-0.734131
31	1	0	1.004336	0.576149	1.930842

### 2c-cis

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.815422	0.156069	1.280711
2	6	0	1.428751	-0.709389	0.079191
3	6	0	0.362088	-1.757921	0.267945
4	6	0	0.339994	-2.825850	-0.792979
5	6	0	-0.491320	-1.770316	1.287573
6	6	0	1.815210	1.631915	-0.617883
7	6	0	1.135608	0.314088	-1.073253
8	6	0	-0.341835	0.481961	-1.442224
9	1	0	1.619187	-0.047478	-1.982795
10	1	0	2.336891	-1.245152	-0.223451
11	1	0	0.928926	0.583732	1.748875
12	1	0	1.051766	2.362024	-0.351444
13	1	0	2.427944	2.063507	-1.410117
14	1	0	-0.734820	-0.413727	-1.922424
15	6	0	-1.272687	0.825598	-0.305240
16	1	0	-0.528103	-3.476497	-0.693886
17	1	0	0.336075	-2.389339	-1.795156
18	1	0	1.243271	-3.438354	-0.722909
19	1	0	-1.246469	-2.543701	1.370411
20	1	0	-0.466312	-1.018614	2.066509
21	8	0	-2.497475	0.322363	-0.515405
22	8	0	-1.006674	1.495913	0.660340
23	6	0	-3.453704	0.580170	0.513609
24	1	0	-4.378137	0.117117	0.182906
25	1	0	-3.118507	0.137984	1.451776
26	1	0	-3.588707	1.652037	0.651135
27	1	0	2.369441	-0.410811	2.030279
28	6	0	2.631582	1.274370	0.632124
29	1	0	2.784228	2.130860	1.288765
30	1	0	3.616481	0.893289	0.347311
31	1	0	-0.434626	1.292740	-2.172712

## 2c-trans

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.032509	-1.238749	-0.790226
2	6	0	-1.223858	0.005612	-0.408423
3	6	0	-0.498842	-0.437121	0.890205
4	6	0	-0.365453	-1.980685	0.791594
5	6	0	-1.992820	1.289710	-0.235484
6	6	0	-3.307746	1.221995	0.492653
7	6	0	0.796345	0.319847	1.147583
8	6	0	-1.509619	2.442318	-0.693319
9	1	0	-1.156436	-0.202154	1.731545
10	1	0	-0.466570	0.156863	-1.181129
11	1	0	-2.893539	-1.347090	-0.123174
12	1	0	0.674333	-2.304848	0.826269
13	1	0	-0.881701	-2.449463	1.631220
14	1	0	0.609512	1.398321	1.157549
15	6	0	1.891256	0.068400	0.140199
16	1	0	-3.681598	2.219098	0.721618
17	1	0	-3.220896	0.661722	1.426929
18	1	0	-4.055388	0.707753	-0.116093
19	1	0	-2.034241	3.378919	-0.543660
20	1	0	-0.574134	2.480430	-1.240746
21	8	0	2.996582	0.760890	0.453382
22	8	0	1.827263	-0.647399	-0.826342
23	6	0	4.102906	0.603377	-0.438259
24	1	0	4.898052	1.222895	-0.035689
25	1	0	4.413086	-0.439871	-0.477228
26	1	0	3.831622	0.932846	-1.440286
27	1	0	-2.402124	-1.201909	-1.815902
28	6	0	-1.036538	-2.371837	-0.536204
29	1	0	-1.506695	-3.354671	-0.498857
30	1	0	-0.289360	-2.380212	-1.331689
31	1	0	1.206580	0.076235	2.131102

**1d**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.567968	-0.306165	-0.279193
2	6	0	-2.926272	0.900561	0.341406
3	6	0	-2.024569	0.931549	1.323147
4	6	0	-1.439990	2.230364	1.802972
5	6	0	-1.467452	-0.281142	2.013211
6	6	0	-1.522804	-1.124958	-1.578924
7	6	0	-0.536774	-0.034405	-1.315620
8	6	0	0.659397	-0.129779	-0.721553
9	6	0	1.506585	1.094178	-0.667710
10	8	0	2.808630	0.806692	-0.601654
11	6	0	3.690385	1.931052	-0.564692
12	8	0	1.083445	2.221586	-0.736125
13	1	0	-0.802094	0.953305	-1.684765
14	1	0	-3.220263	1.852834	-0.096383
15	1	0	-3.483431	-1.178580	0.371243
16	1	0	-1.415066	-1.931895	-0.852308
17	1	0	-1.241616	-1.564684	-2.543139
18	1	0	-0.374307	-0.247114	1.982762
19	6	0	1.142653	-1.411415	-0.141463
20	1	0	-0.367054	2.257154	1.592547
21	1	0	-1.903435	3.086937	1.314851
22	1	0	-1.562649	2.333256	2.884786
23	1	0	-1.753857	-0.285514	3.068794
24	1	0	-1.789382	-1.220451	1.566738
25	1	0	4.691682	1.517621	-0.499903
26	1	0	3.579256	2.528666	-1.468226
27	1	0	3.473994	2.550901	0.304222
28	8	0	1.824291	-1.228542	0.993583
29	8	0	0.910333	-2.502848	-0.599130
30	6	0	2.312260	-2.416447	1.621008
31	1	0	2.858399	-2.083301	2.497643
32	1	0	1.481486	-3.060079	1.907941
33	1	0	2.968595	-2.958978	0.942173
34	1	0	-4.637168	-0.113573	-0.401127
35	6	0	-2.975124	-0.649224	-1.652449
36	1	0	-3.574716	-1.438519	-2.110299
37	1	0	-3.043923	0.221891	-2.311785

**1d'**

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.518404	1.779280	-0.048916
2	6	0	2.661788	0.447342	0.628254
3	6	0	0.001050	1.033571	-1.368190
4	6	0	1.303745	0.665773	-1.995390
5	6	0	1.925206	-0.048567	1.624298
6	6	0	0.786048	0.666907	2.297196
7	6	0	-0.843712	0.258653	-0.683794
8	6	0	-2.054511	0.899988	-0.090716
9	8	0	-3.012042	0.015166	0.183068
10	6	0	-4.204326	0.549585	0.763622
11	8	0	-2.175722	2.086224	0.087694
12	6	0	2.204512	-1.414571	2.190324
13	1	0	-0.276857	2.084275	-1.433890
14	1	0	3.468142	-0.176225	0.242618
15	1	0	1.646248	2.312934	0.331192
16	1	0	1.586154	-0.350501	-1.731495
17	1	0	1.185402	0.697791	-3.083181
18	1	0	1.320705	-2.049282	2.084630
19	6	0	-0.616826	-1.191586	-0.409816
20	1	0	1.048065	0.885889	3.336568
21	1	0	-0.092450	0.017068	2.316079
22	1	0	0.509767	1.600863	1.812765
23	1	0	2.427295	-1.348713	3.259072
24	1	0	3.047127	-1.894263	1.691714

25	1	0	-4.854405	-0.302034	0.935381
26	1	0	-3.971969	1.050785	1.702003
27	1	0	-4.670590	1.259648	0.082189
28	8	0	-0.196767	-1.858711	-1.489667
29	8	0	-0.778946	-1.713712	0.662325
30	6	0	0.133981	-3.233660	-1.267653
31	1	0	0.463282	-3.615953	-2.228481
32	1	0	0.930004	-3.312035	-0.527568
33	1	0	-0.739553	-3.779122	-0.914663
34	1	0	3.386802	2.404314	0.180947
35	6	0	2.405719	1.646667	-1.573933
36	1	0	2.213980	2.631382	-2.007728
37	1	0	3.354202	1.295152	-1.987230

### TSd-*cis*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.125266	-0.794934	0.355968
2	6	0	-2.253327	0.403054	-0.028484
3	6	0	-1.709513	1.257791	0.974626
4	6	0	-1.880427	2.736466	0.890590
5	6	0	-0.836723	0.684084	1.937309
6	6	0	-1.498074	-1.858258	-1.003260
7	6	0	-0.935182	-0.438639	-0.919442
8	6	0	0.422711	-0.262636	-0.422514
9	6	0	0.976502	1.046072	-0.691241
10	8	0	2.317409	1.155979	-0.660600
11	6	0	2.828867	2.469094	-0.868442
12	8	0	0.259667	2.010052	-0.922220
13	1	0	-1.078366	0.117347	-1.844219
14	1	0	-2.754922	0.980232	-0.804407
15	1	0	-2.748110	-1.273768	1.262094
16	1	0	-1.090578	-2.471038	-0.200508
17	1	0	-1.198946	-2.326075	-1.941352
18	1	0	0.027824	0.367808	1.180916
19	6	0	1.283193	-1.384765	-0.019014
20	1	0	-1.040973	3.267500	1.337140
21	1	0	-2.007491	3.060879	-0.139986
22	1	0	-2.785100	3.004530	1.449961
23	1	0	-0.444265	1.344457	2.703852
24	1	0	-1.102219	-0.303222	2.311720
25	1	0	3.909847	2.374800	-0.822166
26	1	0	2.522033	2.853433	-1.840603
27	1	0	2.475299	3.147795	-0.092326
28	8	0	2.180325	-1.039854	0.927659
29	8	0	1.221101	-2.521545	-0.434792
30	6	0	3.138199	-2.040570	1.261390
31	1	0	3.802730	-1.582943	1.988480
32	1	0	2.649378	-2.914988	1.689953
33	1	0	3.696163	-2.345848	0.376482
34	1	0	-4.148109	-0.467386	0.547083
35	6	0	-3.004685	-1.754888	-0.819364
36	1	0	-3.470259	-2.721550	-0.627368
37	1	0	-3.479605	-1.320242	-1.703865

### TSd-*trans*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.311181	-0.391707	-0.341681
2	6	0	2.054076	-0.279648	0.500466
3	6	0	0.909622	-0.113706	-0.709036
4	6	0	1.385072	-1.248958	-1.634019
5	6	0	1.803904	0.835119	1.366159
6	6	0	2.451406	2.153472	1.121150
7	6	0	-0.492818	-0.063948	-0.274360
8	6	0	-1.186903	1.186021	-0.583315

9	8	0	-2.526826	1.149359	-0.540018
10	6	0	-3.180910	2.394518	-0.772558
11	8	0	-0.592394	2.224944	-0.824719
12	6	0	0.666101	0.708791	2.187444
13	1	0	1.151955	0.841942	-1.172825
14	1	0	1.774175	-1.230153	0.957384
15	1	0	3.579741	0.589586	-0.738752
16	1	0	0.912394	-2.182167	-1.338259
17	1	0	1.082145	-1.022361	-2.656300
18	1	0	-0.127334	0.547456	1.252623
19	6	0	-1.094317	-1.303774	0.201865
20	1	0	2.033362	2.930872	1.756316
21	1	0	2.321740	2.447428	0.075067
22	1	0	3.527041	2.080468	1.302941
23	1	0	0.373891	1.557980	2.795181
24	1	0	0.511423	-0.263117	2.654693
25	1	0	-4.243600	2.185648	-0.691150
26	1	0	-2.879917	3.133091	-0.030234
27	1	0	-2.943249	2.775217	-1.765186
28	8	0	-2.434328	-1.342262	0.256863
29	8	0	-0.422126	-2.245973	0.591738
30	6	0	-2.990186	-2.532674	0.810416
31	1	0	-4.066607	-2.390316	0.787613
32	1	0	-2.708870	-3.401781	0.216935
33	1	0	-2.647420	-2.679427	1.834274
34	1	0	4.158954	-0.757519	0.238162
35	6	0	2.921551	-1.344793	-1.488501
36	1	0	3.436889	-1.077316	-2.410217
37	1	0	3.211996	-2.366349	-1.243361

## 2d-cis

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.398126	-2.131222	0.082154
2	6	0	-1.900269	-0.741671	-0.376459
3	6	0	-2.376165	0.387098	0.517994
4	6	0	-3.230920	1.429549	-0.146533
5	6	0	-2.101291	0.435362	1.819091
6	6	0	-0.054936	-2.385937	-0.179652
7	6	0	-0.347206	-0.929212	-0.577501
8	6	0	0.562629	0.070193	0.138704
9	6	0	0.328919	1.485654	-0.350391
10	8	0	0.921650	2.374109	0.451025
11	6	0	0.783088	3.744878	0.063906
12	8	0	-0.287208	1.784907	-1.337195
13	1	0	-0.146476	-0.809230	-1.643816
14	1	0	-2.308091	-0.550325	-1.370559
15	1	0	-2.391041	-2.178448	1.173645
16	1	0	0.162375	-2.441847	0.892204
17	1	0	0.804423	-2.796635	-0.713040
18	1	0	0.414964	0.049805	1.216461
19	6	0	2.007991	-0.293938	-0.147105
20	1	0	-3.537144	2.205687	0.554656
21	1	0	-2.691342	1.887996	-0.977254
22	1	0	-4.129275	0.962968	-0.561258
23	1	0	-2.464800	1.243688	2.442222
24	1	0	-1.520297	-0.336462	2.312719
25	1	0	1.320067	4.318990	0.811979
26	1	0	1.212916	3.901492	-0.924178
27	1	0	-0.269836	4.023607	0.048468
28	8	0	2.573152	-0.930263	0.880726
29	8	0	2.571723	-0.074683	-1.186865
30	6	0	3.913662	-1.384859	0.662830
31	1	0	4.211773	-1.874907	1.583913
32	1	0	3.940569	-2.084174	-0.171802
33	1	0	4.565954	-0.540591	0.446411
34	1	0	-3.417983	-2.326118	-0.250670
35	6	0	-1.366262	-3.111863	-0.469551
36	1	0	-1.422332	-4.097703	-0.008027
37	1	0	-1.495644	-3.234538	-1.548532

## 2d-trans

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.971451	-0.781740	-0.970635
2	6	0	2.031050	-0.300304	0.145689
3	6	0	0.752747	0.039284	-0.646680
4	6	0	0.611839	-1.166327	-1.581324
5	6	0	2.538659	0.828896	1.006265
6	6	0	3.196481	1.997377	0.322328
7	6	0	-0.462484	0.365667	0.230994
8	6	0	-1.547973	1.088239	-0.542833
9	8	0	-2.500398	1.537431	0.279102
10	6	0	-3.606884	2.189839	-0.350380
11	8	0	-1.559487	1.263663	-1.731534
12	6	0	2.370746	0.798604	2.326257
13	1	0	0.945473	0.927614	-1.256216
14	1	0	1.794122	-1.145441	0.798708
15	1	0	3.445568	0.079273	-1.444835
16	1	0	0.185458	-2.007810	-1.027577
17	1	0	-0.045636	-0.960809	-2.424613
18	1	0	-0.143601	1.018635	1.048371
19	6	0	-1.008146	-0.887948	0.886508
20	1	0	3.330615	2.826897	1.015344
21	1	0	2.605414	2.349881	-0.526726
22	1	0	4.178305	1.719077	-0.067324
23	1	0	2.698672	1.617021	2.957039
24	1	0	1.893990	-0.046715	2.809667
25	1	0	-4.276880	2.477188	0.453441
26	1	0	-3.266217	3.066828	-0.898513
27	1	0	-4.102111	1.505203	-1.037665
28	8	0	-2.069063	-1.377739	0.239646
29	8	0	-0.514831	-1.416569	1.847414
30	6	0	-2.599747	-2.604431	0.751258
31	1	0	-3.447317	-2.845544	0.118213
32	1	0	-1.845241	-3.388355	0.699107
33	1	0	-2.914353	-2.474997	1.785411
34	1	0	3.766510	-1.418971	-0.583990
35	6	0	2.060943	-1.503475	-1.994316
36	1	0	2.269815	-1.154883	-3.005542
37	1	0	2.225553	-2.580467	-1.988121

## 1e

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.812237	1.466991	0.382150
2	6	0	2.000539	0.120275	-0.255387
3	6	0	1.573815	-1.064108	0.178642
4	6	0	0.768507	-1.276587	1.428674
5	6	0	-0.643808	2.044483	-0.144827
6	6	0	-1.075257	0.733216	-0.738526
7	6	0	-1.917450	-0.164112	-0.228900
8	6	0	1.836019	-2.321543	-0.604357
9	1	0	2.546922	0.139920	-1.197238
10	1	0	1.482202	1.373580	1.418560
11	1	0	-0.846392	2.074226	0.928182
12	1	0	-1.243588	2.845483	-0.592078
13	1	0	-0.135348	-1.842546	1.185839
14	1	0	2.456302	-2.130822	-1.479760
15	1	0	2.334169	-3.070860	0.017300
16	1	0	0.891695	-2.762893	-0.937972
17	1	0	1.332706	-1.869079	2.154935
18	1	0	0.456808	-0.347428	1.901467
19	1	0	2.786484	1.963766	0.414922
20	6	0	0.834136	2.377312	-0.376218
21	1	0	1.0544853	2.334658	-1.448038
22	1	0	1.0044300	3.410691	-0.064592
23	1	0	-0.644384	0.515009	-1.714120
24	6	0	-2.245634	-1.428901	-0.976216

25	1	0	-1.713268	-1.484018	-1.925696
26	1	0	-1.980536	-2.308682	-0.381063
27	1	0	-3.319032	-1.497312	-1.175704
28	6	0	-2.614986	-0.034971	1.097036
29	1	0	-3.698564	-0.002876	0.950266
30	1	0	-2.408378	-0.908730	1.721989
31	1	0	-2.325657	0.855585	1.650388

1e'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.730778	0.726826	-0.016916
2	6	0	-1.730934	0.726588	0.016900
3	6	0	-0.970919	1.703675	-0.830323
4	6	0	0.970575	1.703736	0.830346
5	6	0	-1.831439	-0.592973	-0.143383
6	6	0	1.831537	-0.592717	0.143348
7	6	0	2.627476	-1.434441	-0.816883
8	6	0	1.206677	-1.371463	1.268975
9	1	0	-2.245368	1.166911	0.870935
10	1	0	2.245158	1.167274	-0.870918
11	1	0	0.414923	1.185162	1.611661
12	1	0	-0.415231	1.185245	-1.611708
13	1	0	-1.674721	2.372401	-1.336482
14	1	0	1.978880	-2.166580	-1.307947
15	1	0	0.742374	-2.282835	0.883304
16	1	0	0.447227	-0.810009	1.808312
17	1	0	1.975397	-1.688206	1.980345
18	1	0	3.399963	-2.000423	-0.288468
19	1	0	3.107235	-0.828320	-1.585044
20	1	0	1.674265	2.372513	1.336596
21	6	0	-0.000215	2.552918	0.000035
22	1	0	-0.565203	3.205427	0.671805
23	1	0	0.564695	3.205531	-0.671699
24	6	0	-2.627130	-1.434872	0.816902
25	1	0	-1.978336	-2.166877	1.307905
26	1	0	-3.106949	-0.828859	1.585112
27	1	0	-3.399546	-2.001008	0.288550
28	6	0	-1.206481	-1.371599	-1.269028
29	1	0	-0.741483	-2.282584	-0.883272
30	1	0	-1.975261	-1.689000	-1.980045
31	1	0	-0.447567	-0.809821	-1.808780

### TSe-cis

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.677584	-1.344367	0.548542
2	6	0	0.385633	-1.429002	-0.221388
3	6	0	-0.897744	-1.519779	0.299935
4	6	0	-1.246546	-0.754668	1.421388
5	6	0	1.933687	0.873186	-0.428118
6	6	0	0.469609	0.687425	-0.760490
7	6	0	-0.548530	1.395011	-0.081899
8	6	0	-2.001773	-2.051949	-0.583157
9	1	0	0.522623	-1.891827	-1.198308
10	1	0	1.522064	-0.904943	1.537090
11	1	0	2.035381	1.436112	0.500179
12	1	0	2.413319	1.469487	-1.209973
13	1	0	-1.037323	0.452943	0.775052
14	1	0	-1.752993	-1.933984	-1.640209
15	1	0	-2.162866	-3.118112	-0.403569
16	1	0	-2.946843	-1.540384	-0.393277
17	1	0	-2.272027	-0.783482	1.775612
18	1	0	-0.513301	-0.583083	2.204103
19	1	0	2.087187	-2.347648	0.696597
20	6	0	2.636480	-0.473472	-0.255594
21	1	0	2.808287	-0.938190	-1.231342

22	1	0	3.607547	-0.362082	0.230006
23	1	0	0.263925	0.425478	-1.794228
24	6	0	-1.821295	1.647919	-0.874491
25	1	0	-2.070358	0.777978	-1.485924
26	1	0	-2.667741	1.849582	-0.213923
27	1	0	-1.705727	2.507066	-1.542606
28	6	0	-0.208975	2.493208	0.913647
29	1	0	0.254174	3.355478	0.423819
30	1	0	-1.121224	2.839317	1.403453
31	1	0	0.467119	2.149220	1.697193

### TSe-trans

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.105816	0.259236	-0.652494
2	6	0	0.272812	-0.723590	0.501200
3	6	0	-0.353801	-2.038674	0.096900
4	6	0	-2.293308	-0.449517	-0.064160
5	6	0	1.568645	-0.293790	0.168375
6	6	0	-0.723820	1.575689	-0.454073
7	6	0	0.515842	1.921218	-1.044934
8	6	0	-1.254632	2.364402	0.712088
9	1	0	-0.082457	-0.379911	1.474251
10	1	0	-0.745745	-0.184174	-1.580347
11	1	0	-2.590080	0.039678	0.865506
12	1	0	-0.060647	-2.292774	-0.923383
13	1	0	0.017421	-2.844668	0.736986
14	1	0	1.239533	0.994173	-0.448181
15	1	0	-0.803217	3.355019	0.753347
16	1	0	-1.040154	1.856952	1.660527
17	1	0	-2.337479	2.488321	0.653609
18	1	0	0.934129	2.901956	-0.837755
19	1	0	0.693379	1.584495	-2.064681
20	1	0	-3.152662	-0.401580	-0.736449
21	6	0	-1.885589	-1.921897	0.207137
22	1	0	-2.211656	-2.216845	1.205487
23	1	0	-2.371032	-2.601857	-0.493535
24	6	0	2.437873	0.293902	1.264608
25	1	0	3.216255	0.940714	0.852108
26	1	0	1.839124	0.887364	1.958748
27	1	0	2.934659	-0.494237	1.840814
28	6	0	2.317211	-1.000725	-0.939036
29	1	0	3.187016	-0.417345	-1.248241
30	1	0	2.674582	-1.986670	-0.622727
31	1	0	1.686526	-1.146137	-1.819749

### 2e-cis

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.322376	1.752308	-0.341724
2	6	0	0.808496	0.295089	-0.566680
3	6	0	1.573927	-0.691586	0.296142
4	6	0	1.451591	-0.752615	1.618553
5	6	0	-0.957753	1.698988	0.404631
6	6	0	-0.744665	0.391863	-0.366984
7	6	0	-1.472336	-0.838306	0.177276
8	6	0	2.564712	-1.551976	-0.439447
9	1	0	0.989833	0.009902	-1.605134
10	1	0	1.875958	1.788306	0.597506
11	1	0	-0.741618	1.552649	1.468802
12	1	0	-1.977673	2.075078	0.320151
13	1	0	-1.080824	-1.072016	1.170201
14	1	0	2.067688	-2.154834	-1.204271
15	1	0	3.291580	-0.921977	-0.960943
16	1	0	3.103083	-2.217005	0.235058
17	1	0	2.040664	-1.445417	2.207879

18	1	0	0.769844	-0.106450	2.159599
19	1	0	1.998438	2.077803	-1.132776
20	6	0	0.072915	2.632918	-0.224843
21	1	0	-0.276407	2.937222	-1.215231
22	1	0	0.255086	3.538070	0.355127
23	1	0	-1.153986	0.564124	-1.371951
24	6	0	-1.238366	-2.047290	-0.725836
25	1	0	-0.179959	-2.302502	-0.788450
26	1	0	-1.772102	-2.923447	-0.352720
27	1	0	-1.599372	-1.839917	-1.737787
28	6	0	-2.971147	-0.565699	0.309119
29	1	0	-3.390883	-0.253229	-0.651894
30	1	0	-3.499167	-1.466736	0.627226
31	1	0	-3.178679	0.218214	1.038367

## 2e-trans

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.763355	0.361250	-0.380995
2	6	0	-0.570970	0.251437	0.374345
3	6	0	-1.290458	1.553116	-0.015905
4	6	0	1.161984	1.818865	-0.107522
5	6	0	-1.349850	-1.051216	0.159196
6	6	0	1.792267	-0.675045	-0.013288
7	6	0	2.399154	-1.403047	-0.947326
8	6	0	2.095277	-0.865800	1.448751
9	1	0	-0.340088	0.317070	1.445631
10	1	0	0.556213	0.274139	-1.453253
11	1	0	1.555275	1.906757	0.907998
12	1	0	-1.853449	1.406672	-0.940404
13	1	0	-2.004772	1.865920	0.745867
14	1	0	-0.746572	-1.855875	0.596526
15	1	0	2.931658	-1.549740	1.587142
16	1	0	1.228848	-1.277339	1.973071
17	1	0	2.341025	0.081376	1.933646
18	1	0	3.147096	-2.144976	-0.692523
19	1	0	2.166076	-1.275935	-1.998622
20	1	0	1.933056	2.173463	-0.791694
21	6	0	-0.164558	2.596816	-0.234436
22	1	0	-0.219067	3.410793	0.488155
23	1	0	-0.248624	3.045410	-1.224789
24	6	0	-2.685081	-1.005596	0.901333
25	1	0	-3.184905	-1.975383	0.868776
26	1	0	-2.546821	-0.728631	1.949086
27	1	0	-3.353409	-0.270560	0.445467
28	6	0	-1.564685	-1.399733	-1.313211
29	1	0	-2.167739	-2.305650	-1.399900
30	1	0	-2.093632	-0.602337	-1.840802
31	1	0	-0.618779	-1.581453	-1.825030

## 1f

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.996021	-1.069674	1.214304
2	6	0	-3.003225	-0.322147	0.391423
3	6	0	-3.011768	0.972655	0.071981
4	6	0	-1.985356	1.981251	0.510405
5	6	0	-0.713090	-1.796186	-0.883483
6	6	0	0.238070	-0.657374	-0.680028
7	6	0	1.527674	-0.750001	-0.348715
8	6	0	2.258172	0.537486	-0.159185
9	8	0	1.781167	1.642346	-0.255063
10	6	0	-4.105935	1.549464	-0.785988
11	8	0	3.549833	0.336854	0.144532
12	6	0	4.328565	1.517126	0.346279
13	1	0	-3.813793	-0.936888	0.000878
14	1	0	-1.207446	-0.405454	1.568861

15	1	0	-0.210548	-2.651259	-1.338097
16	1	0	-1.495866	-1.474661	-1.573026
17	1	0	-1.537636	2.468514	-0.360375
18	1	0	-3.687455	1.998207	-1.691163
19	1	0	-4.831912	0.791546	-1.078922
20	1	0	-4.632568	2.346258	-0.253390
21	1	0	-2.464405	2.768722	1.098907
22	1	0	-1.178367	1.556796	1.102996
23	1	0	5.331247	1.173779	0.581002
24	1	0	4.333491	2.126527	-0.556370
25	1	0	3.921445	2.103309	1.168997
26	1	0	-2.485486	-1.475920	2.104739
27	6	0	-1.365435	-2.234412	0.438625
28	1	0	-2.128021	-2.986561	0.218887
29	1	0	-0.611804	-2.713232	1.069436
30	1	0	-0.172897	0.343614	-0.773853
31	6	0	2.286991	-2.028594	-0.141628
32	1	0	3.135080	-2.094227	-0.824696
33	1	0	2.691041	-2.076132	0.870777
34	1	0	1.646048	-2.894110	-0.295282

## 1f'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.538606	0.519045	-0.279515
2	6	0	0.024270	-1.644285	0.304583
3	6	0	1.369647	-1.962137	0.869963
4	6	0	2.435649	-0.732956	-1.099917
5	6	0	-0.811900	-0.676086	0.685998
6	6	0	-2.066549	-0.541513	-0.112160
7	8	0	-2.380585	-1.222452	-1.058433
8	6	0	1.730189	1.579521	-0.294457
9	6	0	1.980075	2.756106	0.610276
10	6	0	0.536164	1.742107	-1.195118
11	8	0	-2.837016	0.463540	0.333524
12	6	0	-4.048957	0.680860	-0.390330
13	1	0	-0.292023	-2.254722	-0.538646
14	1	0	3.378286	0.541239	0.414854
15	1	0	1.532531	-0.721485	-1.710735
16	1	0	1.655062	-1.235522	1.629520
17	1	0	1.330957	-2.940882	1.358448
18	1	0	1.124406	2.919933	1.271999
19	1	0	-0.345484	2.019766	-0.609607
20	1	0	0.294357	0.845318	-1.760522
21	1	0	0.711215	2.557787	-1.902728
22	1	0	2.107984	3.672105	0.026668
23	1	0	2.868115	2.611328	1.225075
24	1	0	-4.539165	1.517718	0.097305
25	1	0	-3.830428	0.917490	-1.430912
26	1	0	-4.677907	-0.207395	-0.351840
27	1	0	3.280343	-0.786254	-1.793919
28	6	0	2.439092	-1.998543	-0.231806
29	1	0	2.277656	-2.869226	-0.872521
30	1	0	3.418610	-2.125510	0.236233
31	6	0	-0.604409	0.280055	1.824764
32	1	0	-0.773005	1.307652	1.503059
33	1	0	-1.315555	0.080259	2.629041
34	1	0	0.403607	0.208653	2.224814

## TSf-cis

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.627797	-0.210575	0.730279
2	6	0	-1.863883	0.773747	-0.133019
3	6	0	-1.031675	1.781584	0.388235
4	6	0	-0.283197	1.472072	1.549716
5	6	0	-1.707985	-1.523590	-1.154417

6	6	0	-0.661344	-0.446946	-0.850626
7	6	0	0.416706	-0.782740	0.032391
8	6	0	1.694825	-0.174331	-0.300103
9	8	0	1.836969	0.836030	-0.967346
10	6	0	-0.629936	2.906347	-0.516924
11	8	0	2.753977	-0.809399	0.255933
12	6	0	4.022640	-0.205209	0.021415
13	1	0	-2.415594	1.061532	-1.028653
14	1	0	-2.034578	-0.472016	1.606914
15	1	0	-1.238973	-2.507999	-1.168010
16	1	0	-2.095412	-1.343761	-2.157255
17	1	0	0.264836	0.448546	1.098618
18	1	0	-0.268404	2.508648	-1.470168
19	1	0	-1.486701	3.551441	-0.726914
20	1	0	0.164410	3.509586	-0.081253
21	1	0	0.469075	2.192508	1.855765
22	1	0	-0.806841	1.025218	2.390589
23	1	0	4.749176	-0.832698	0.529812
24	1	0	4.238174	-0.164178	-1.045729
25	1	0	4.047205	0.806931	0.424704
26	1	0	-3.563113	0.223917	1.087736
27	6	0	-2.863814	-1.459681	-0.128515
28	1	0	-3.819772	-1.387351	-0.648568
29	1	0	-2.908535	-2.356772	0.490043
30	1	0	-0.326260	0.108921	-1.721901
31	6	0	0.392979	-2.041538	0.863833
32	1	0	0.711480	-2.915582	0.286005
33	1	0	1.059862	-1.960868	1.721051
34	1	0	-0.612730	-2.243906	1.234932

### TSf-trans

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.837238	0.342685	0.537560
2	6	0	0.618959	-0.688642	-0.329692
3	6	0	1.528399	-1.909097	-0.390313
4	6	0	3.029554	0.067174	-0.351756
5	6	0	-0.655975	-0.754275	0.312958
6	6	0	-1.751777	-0.114715	-0.393509
7	8	0	-1.631284	0.719184	-1.276072
8	6	0	1.184382	1.586379	0.641194
9	6	0	0.132619	1.617734	1.592994
10	6	0	1.265668	2.588816	-0.466166
11	8	0	-2.974658	-0.492057	0.053393
12	6	0	-4.079352	0.168142	-0.556672
13	1	0	0.567297	-0.179673	-1.291954
14	1	0	1.879513	-0.202243	1.482409
15	1	0	2.990932	0.715766	-1.228272
16	1	0	1.546470	-2.401880	0.583222
17	1	0	1.135644	-2.630538	-1.109170
18	1	0	-0.530370	0.680599	1.135279
19	1	0	0.580392	3.417547	-0.299427
20	1	0	1.006522	2.122091	-1.422665
21	1	0	2.279520	2.985107	-0.560167
22	1	0	-0.478716	2.513547	1.641120
23	1	0	0.353223	1.192705	2.571518
24	1	0	-4.968190	-0.247074	-0.089970
25	1	0	-4.028167	1.243291	-0.385602
26	1	0	-4.093718	-0.016502	-1.630253
27	1	0	3.962916	0.284342	0.169062
28	6	0	2.935377	-1.418870	-0.777410
29	1	0	3.090913	-1.511954	-1.852172
30	1	0	3.702972	-2.021642	-0.292669
31	6	0	-0.915406	-1.764919	1.397593
32	1	0	-1.844167	-1.547831	1.921056
33	1	0	-0.980561	-2.785859	1.008458
34	1	0	-0.103004	-1.749290	2.130941

### 2f-cis

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.345965	-1.212356	0.564324
2	6	0	-1.867391	-0.164438	-0.440817
3	6	0	-2.178143	1.285091	-0.175763
4	6	0	-2.714986	1.725435	0.958040
5	6	0	-0.273114	-2.026061	-0.436550
6	6	0	-0.361883	-0.493588	-0.663721
7	6	0	0.604592	0.309487	0.221387
8	6	0	2.031313	0.042482	-0.226465
9	8	0	2.361248	-0.669397	-1.140572
10	6	0	-1.881013	2.214101	-1.322930
11	8	0	2.922927	0.725093	0.507462
12	6	0	4.292423	0.556830	0.135342
13	1	0	-2.356648	-0.410360	-1.393248
14	1	0	-2.007157	-0.972572	1.573496
15	1	0	0.502091	-2.260257	0.293907
16	1	0	0.014625	-2.537116	-1.353930
17	1	0	0.448633	1.377873	0.031787
18	1	0	-0.843708	2.121875	-1.654435
19	1	0	-2.507315	1.958421	-2.182071
20	1	0	-2.068403	3.253475	-1.056004
21	1	0	-2.932812	2.777205	1.102514
22	1	0	-2.963649	1.055942	1.772434
23	1	0	4.864010	1.171561	0.823594
24	1	0	4.583178	-0.488957	0.223861
25	1	0	4.449111	0.884613	-0.891437
26	1	0	-3.433615	-1.293564	0.589844
27	6	0	-1.659210	-2.486588	0.064864
28	1	0	-2.235895	-2.903924	-0.763639
29	1	0	-1.589382	-3.258160	0.831789
30	1	0	-0.094528	-0.260673	-1.694986
31	6	0	0.458971	0.107039	1.734407
32	1	0	0.524970	-0.946701	2.009502
33	1	0	1.241834	0.647221	2.263505
34	1	0	-0.502306	0.493918	2.065680

## 2f-trans

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.794877	-0.035046	0.338981
2	6	0	0.399352	-0.515746	-0.089681
3	6	0	0.437577	-1.994038	0.300005
4	6	0	2.713088	-1.170256	-0.164537
5	6	0	-0.752388	0.323132	0.462109
6	6	0	-2.042019	-0.001556	-0.266842
7	8	0	-2.151729	-0.754395	-1.200925
8	6	0	2.166731	1.344176	-0.139302
9	6	0	2.642716	2.258494	0.702218
10	6	0	1.956135	1.650592	-1.597705
11	8	0	-3.084863	0.672504	0.238774
12	6	0	-4.342416	0.444840	-0.401487
13	1	0	0.348949	-0.469889	-1.182769
14	1	0	1.834766	-0.035697	1.432564
15	1	0	3.062043	-0.951047	-1.174860
16	1	0	0.355864	-2.089102	1.386002
17	1	0	-0.370866	-2.567565	-0.152315
18	1	0	-0.545761	1.374902	0.224615
19	1	0	2.399015	2.609399	-1.863668
20	1	0	0.889100	1.691947	-1.833578
21	1	0	2.389792	0.878952	-2.237190
22	1	0	2.923846	3.249387	0.364772
23	1	0	2.770323	2.039542	1.756392
24	1	0	-5.060594	1.062237	0.128870
25	1	0	-4.291140	0.732568	-1.450658
26	1	0	-4.617050	-0.606802	-0.332888
27	1	0	3.597694	-1.263291	0.464811
28	6	0	1.834863	-2.449365	-0.161417
29	1	0	1.778170	-2.869221	-1.166274

30	1	0	2.241926	-3.224646	0.486976
31	6	0	-0.946953	0.225275	1.978834
32	1	0	-1.688427	0.946815	2.315368
33	1	0	-1.285172	-0.769834	2.270429
34	1	0	-0.009122	0.433467	2.493547

## 1g

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.738478	-0.921662	-0.836953
2	6	0	2.671377	0.442106	-0.211397
3	6	0	1.789897	1.412546	-0.451084
4	6	0	0.642121	1.306792	-1.414956
5	6	0	0.735117	-2.054099	0.291052
6	6	0	0.241856	-0.939980	1.162728
7	6	0	-0.899456	-0.245780	1.101861
8	6	0	-1.898223	-0.507414	0.034339
9	8	0	-1.960583	-1.483310	-0.675551
10	6	0	1.862805	2.726099	0.278477
11	8	0	-2.779674	0.504267	-0.071140
12	6	0	-3.776741	0.351244	-1.081113
13	1	0	3.438566	0.638483	0.535904
14	1	0	2.166074	-0.958869	-1.765766
15	1	0	0.227455	-2.048921	-0.672466
16	1	0	0.448052	-2.996089	0.772864
17	1	0	-0.284653	1.606179	-0.914878
18	1	0	2.734179	2.778512	0.930619
19	1	0	1.907539	3.559443	-0.428281
20	1	0	0.965088	2.873895	0.885941
21	1	0	0.782737	1.991153	-2.256629
22	1	0	0.499722	0.300470	-1.805325
23	1	0	-4.400350	1.237634	-1.018276
24	1	0	-3.312300	0.278975	-2.064015
25	1	0	-4.366559	-0.546278	-0.899987
26	1	0	3.778769	-1.122627	-1.107836
27	6	0	2.253107	-2.044693	0.091390
28	1	0	2.757662	-1.964617	1.060145
29	1	0	2.548933	-3.004596	-0.337397
30	1	0	0.922308	-0.665050	1.966977
31	6	0	-1.201457	0.872666	2.063570
32	1	0	-0.403396	0.958736	2.799962
33	1	0	-1.296537	1.824514	1.537972
34	1	0	-2.144519	0.704440	2.586513

## 1g'

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.498127	0.906023	-1.029404
2	6	0	-0.388307	-1.574991	0.836610
3	6	0	-1.239346	-1.960455	-0.334632
4	6	0	-2.694865	-0.002224	-1.160824
5	6	0	0.817817	-1.003162	0.910780
6	6	0	1.569803	-0.595943	-0.307952
7	8	0	1.310128	-0.871715	-1.454424
8	6	0	-1.184679	1.639609	0.035515
9	6	0	0.097844	2.419803	0.096961
10	6	0	-2.017070	1.685818	1.285632
11	8	0	2.640405	0.153236	0.013915
12	6	0	3.425559	0.611095	-1.085830
13	1	0	-0.853906	-1.802576	1.795550
14	1	0	-0.799923	0.902794	-1.861468
15	1	0	-3.618053	0.534994	-0.924451
16	1	0	-0.737122	-1.759850	-1.276863
17	1	0	-1.388417	-3.042755	-0.266998
18	1	0	0.721245	2.061391	0.922544
19	1	0	-2.094629	2.708476	1.662397
20	1	0	-1.538123	1.089481	2.070883
21	1	0	-3.023156	1.297184	1.132989

22	1	0	-0.093306	3.481052	0.278517
23	1	0	0.668426	2.321714	-0.827468
24	1	0	4.237617	1.185931	-0.651510
25	1	0	3.813394	-0.233577	-1.653643
26	1	0	2.825270	1.236348	-1.746299
27	1	0	-2.778900	-0.311501	-2.204582
28	6	0	-2.617529	-1.265161	-0.286535
29	1	0	-2.854055	-1.010049	0.750269
30	1	0	-3.391903	-1.960372	-0.616655
31	6	0	1.463149	-0.705119	2.239565
32	1	0	1.621280	0.366295	2.371889
33	1	0	0.832869	-1.067606	3.050564
34	1	0	2.441629	-1.181292	2.319090

### TSg-*cis*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.460994	1.578502	-0.952028
2	6	0	-2.020641	0.421864	-0.154553
3	6	0	-2.113329	-0.889331	-0.637920
4	6	0	-1.072438	-1.358967	-1.471988
5	6	0	-0.369175	1.848092	1.240581
6	6	0	-0.553395	0.331390	1.088770
7	6	0	0.500410	-0.526517	0.641632
8	6	0	1.670693	0.048290	-0.012171
9	8	0	1.710180	1.108278	-0.608124
10	6	0	-3.025760	-1.860499	0.055944
11	8	0	2.759312	-0.752650	0.063858
12	6	0	3.917986	-0.278947	-0.617302
13	1	0	-2.824392	0.721841	0.518787
14	1	0	-0.598883	1.256867	-1.534835
15	1	0	0.690276	2.081764	1.312568
16	1	0	-0.833952	2.144600	2.181599
17	1	0	-0.135219	-1.131523	-0.651399
18	1	0	-3.149070	-1.602611	1.110750
19	1	0	-4.019666	-1.837409	-0.399935
20	1	0	-2.654486	-2.883113	-0.016703
21	1	0	-1.082375	-2.411814	-1.737608
22	1	0	-0.729305	-0.717117	-2.278424
23	1	0	4.681425	-1.036605	-0.465875
24	1	0	3.714094	-0.151499	-1.680104
25	1	0	4.243087	0.675308	-0.204319
26	1	0	-2.212954	1.975297	-1.638062
27	6	0	-1.007578	2.620553	0.065865
28	1	0	-1.869888	3.192289	0.416318
29	1	0	-0.303104	3.323627	-0.376554
30	1	0	-1.089458	-0.111305	1.925253
31	6	0	0.619463	-1.877274	1.318011
32	1	0	-0.376463	-2.318982	1.412018
33	1	0	1.242456	-2.564226	0.747950
34	1	0	1.040475	-1.793361	2.323659

### TSg-*trans*

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.574174	0.050380	-0.718860
2	6	0	0.543314	0.493171	0.736306
3	6	0	0.708645	1.994314	0.509783
4	6	0	2.744629	0.979762	-0.482625
5	6	0	-0.722158	-0.171470	0.781605
6	6	0	-1.770059	0.264778	-0.118928
7	8	0	-1.604918	0.897999	-1.149441
8	6	0	1.648089	-1.350539	-0.652609
9	6	0	0.437087	-2.020525	-0.983286
10	6	0	2.733638	-2.042424	0.113699
11	8	0	-3.002288	-0.170558	0.243087

12	6	0	-4.055302	0.147474	-0.661649
13	1	0	1.179997	0.173792	1.565786
14	1	0	0.878781	0.414054	-1.475312
15	1	0	3.493172	0.493583	0.144813
16	1	0	0.079390	2.302781	-0.322309
17	1	0	0.379415	2.533678	1.400131
18	1	0	-0.292334	-1.473450	-0.165439
19	1	0	2.499172	-3.094347	0.268460
20	1	0	2.892460	-1.574123	1.090160
21	1	0	3.684383	-1.980727	-0.422425
22	1	0	0.408026	-3.098746	-0.857500
23	1	0	-0.064668	-1.678774	-1.888340
24	1	0	-4.956955	-0.276687	-0.228944
25	1	0	-4.158217	1.226890	-0.768929
26	1	0	-3.864880	-0.286486	-1.643009
27	1	0	3.230060	1.218113	-1.429887
28	6	0	2.193159	2.249279	0.214532
29	1	0	2.736434	2.427333	1.143577
30	1	0	2.322432	3.137037	-0.403630
31	6	0	-1.062795	-1.020264	1.985283
32	1	0	-1.847487	-1.741827	1.762515
33	1	0	-0.175436	-1.570368	2.309460
34	1	0	-1.400636	-0.414868	2.832148

## 2g-cis

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.587021	1.830281	0.403563
2	6	0	1.692053	0.575696	-0.479991
3	6	0	2.623986	-0.519653	-0.031298
4	6	0	3.245065	-0.533919	1.144760
5	6	0	-0.383369	1.562246	-1.034982
6	6	0	0.209674	0.179269	-0.723912
7	6	0	-0.432785	-0.486103	0.516834
8	6	0	-1.917987	-0.212103	0.541084
9	8	0	-2.490347	0.472160	1.351276
10	6	0	2.852440	-1.605443	-1.049423
11	8	0	-2.555098	-0.816876	-0.472875
12	6	0	-3.961341	-0.575847	-0.555511
13	1	0	2.057609	0.897187	-1.463987
14	1	0	1.580359	1.560198	1.459663
15	1	0	-1.473882	1.588987	-1.032630
16	1	0	-0.059263	1.856728	-2.035528
17	1	0	-0.042682	-0.016729	1.422430
18	1	0	1.909451	-2.061523	-1.360160
19	1	0	3.314048	-1.186975	-1.947883
20	1	0	3.502385	-2.388479	-0.660103
21	1	0	3.914061	-1.345490	1.406775
22	1	0	3.122318	0.251634	1.878093
23	1	0	-4.308333	-1.134376	-1.419162
24	1	0	-4.458929	-0.920396	0.349721
25	1	0	-4.154274	0.488787	-0.685198
26	1	0	2.442524	2.487913	0.250010
27	6	0	0.239688	2.491316	0.022171
28	1	0	0.366827	3.504911	-0.356259
29	1	0	-0.413073	2.551197	0.894241
30	1	0	0.101916	-0.496726	-1.574903
31	6	0	-0.192719	-1.997981	0.585146
32	1	0	0.863097	-2.210233	0.737087
33	1	0	-0.745816	-2.438592	1.416539
34	1	0	-0.525135	-2.476858	-0.336596

## 2g-trans

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.281146	0.329537	-0.460783

2	6	0	-0.739104	-0.715042	0.534130
3	6	0	-1.069365	-2.053317	-0.150405
4	6	0	-2.645584	-0.272432	-0.812328
5	6	0	0.703285	-0.496461	0.991757
6	6	0	1.672397	-0.269024	-0.147229
7	8	0	1.612643	-0.760286	-1.246620
8	6	0	-1.264351	1.743035	0.056152
9	6	0	-0.417872	2.638585	-0.446929
10	6	0	-2.205666	2.091531	1.176608
11	8	0	2.676235	0.539257	0.224301
12	6	0	3.677884	0.781201	-0.765912
13	1	0	-1.350362	-0.648335	1.442521
14	1	0	-0.654195	0.283582	-1.356118
15	1	0	-3.335457	-0.128963	0.023434
16	1	0	-0.241885	-2.350252	-0.793882
17	1	0	-1.226358	-2.848455	0.579074
18	1	0	0.736336	0.410632	1.599852
19	1	0	-2.019955	3.100106	1.543591
20	1	0	-2.101515	1.396850	2.014015
21	1	0	-3.244312	2.034953	0.842938
22	1	0	-0.368768	3.651921	-0.065479
23	1	0	0.250942	2.382080	-1.261706
24	1	0	4.403845	1.438938	-0.298423
25	1	0	4.146591	-0.154033	-1.069225
26	1	0	3.236176	1.258763	-1.639772
27	1	0	-3.093149	0.183646	-1.695819
28	6	0	-2.339872	-1.772147	-0.996022
29	1	0	-3.182073	-2.393699	-0.692816
30	1	0	-2.144355	-1.987649	-2.046835
31	6	0	1.218931	-1.668615	1.837757
32	1	0	2.208556	-1.455539	2.242228
33	1	0	0.536938	-1.848011	2.670288
34	1	0	1.274746	-2.579410	1.239906

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Full reference 14:

Gaussian 16, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.